

## Nanoscale Science Research Centers

### Portfolio Description

The Nanoscale Science Research Centers (NSRCs) are DOE's premier user centers for interdisciplinary research at the nanoscale, serving as the basis for a national program that encompasses new science, new tools, and new computing capabilities. Each center has particular expertise and capabilities in selected theme areas, such as synthesis and characterization of nanomaterials; catalysis; theory, modeling and simulation; electronic materials; nanoscale photonics; soft and biological materials; imaging and spectroscopy; and nanoscale integration. The centers are housed in recently-constructed and custom designed laboratory buildings near one or more other major BES facilities for x-ray, neutron, or electron scattering, which complement and leverage the capabilities of the NSRCs. These laboratories contain clean rooms, nanofabrication resources, one-of-a-kind signature instruments, and other instruments not generally available except at major user facilities. These facilities are routinely made available to the research community during normal working hours. In FY 2011 funds are provided to continue operations for all five NSRCs.

### Unique Aspects

Nanotechnology is the understanding and control of matter at dimensions of roughly 1 to 100 nanometers, where unique phenomena enable novel applications. With a nanometer corresponding to one billionth of a meter, nanoscale phenomena occur at the level of small numbers of atoms, molecules, and supramolecular structures. The NSRCs make sophisticated research tools for nanoscience and nanotechnology available to the broad scientific community, and facilitate access to other collocated major facilities including synchrotron radiation light sources, neutron scattering centers, and electron beam microcharacterization facilities. The NSRCs are the DOE signature activity in nanoscale research and constitute the nation's largest scientific infrastructure investment under the National Nanotechnology Initiative (NNI).

NSRCs provide unique scientific and engineering capabilities not available in any of the parallel programs sponsored by other entities. For example, other federal agencies sponsor research in nanoscience at universities, but such programs are generally limited in scope and size, are focused on specific research issues or topical areas, and primarily involve researchers of the host institution and a limited number of partners. The NSRCs are larger-scale facilities with a broad range of capabilities and are broadly accessible without usage fees for non-proprietary work, with instrument time and staff support allocated on the basis of peer-review of proposals. The purposes of the NSRCs are as follows:

- Advance the fundamental understanding and control of materials at the nanoscale regime.
- Provide an environment to support research of a scope, complexity, and disciplinary breadth not possible under traditional individual investigator or small group efforts.
- Provide the foundation for the development of nanotechnologies important to DOE.
- Provide state-of-the-art equipment to in-house laboratory, university, and industry researchers and leverage the capabilities of national user facilities for materials characterization employing electrons, photons, and neutrons.
- Provide a formal mechanism for both short- and long-term collaborations and partnerships

among DOE laboratory, academic, and industrial researchers.

- Provide training for graduate students and postdoctoral associates in interdisciplinary nanoscale science, engineering, and technology research.

### **Relationship to Other Programs**

The fundamental science being carried out at the NSRCs is closely related to BES programmatic research on the nanometer scale at both universities and national laboratories. Researchers supported by BES, by other parts of the Office of Science, by other parts of DOE, and by other federal agencies as well as industry participate in the overall NSRC user community. While not a requirement, a major benefit is the opportunity for users to collaborate with the NSRC scientists. In addition, the NSRCs are collocated with, and serve as access points to, existing major BES user facilities for x-ray, neutron, and electron scattering. The DOE nanoscience activities as a whole are coordinated with other agencies through the Nanoscale Science, Engineering, and Technology (NSET) Subcommittee of the National Science and Technology Council (NSTC); this Subcommittee is responsible for the federal NNI program and is currently co-chaired by representatives from BES and the Office of Science and Technology Policy (OSTP).

### **Significant Accomplishments**

Physical construction of six new buildings has been completed for the five NSRCs, the initial complement of technical equipment has been successfully installed and commissioned, and all five facilities entered full user operations between FY 2006 and FY 2008. All five had robust pre-operations "jump-start" user programs in which existing capabilities of the host laboratories were made available to outside users as a prelude to operations of the NSRCs themselves. Hundreds of user proposals were accommodated during this period, leading to substantial advances in a number of areas; a few examples include the development and application of methods for the controlled synthesis of hollow or filled nanospheres; new insights on charge transport within two-dimensional and quasi-one-dimensional nanocrystal arrays; and the development of modular microlaboratories that facilitate sophisticated, reproducible measurement of the behavior and properties of nanomaterials. In the operations phase of the NSRCs, user activity has picked up accordingly, with nearly 800 unique users in FY 2007 for the four centers that had operations funding that year. Currently, the facilities have increased substantially their user base and new and exciting discoveries have emerged. Research highlights include the DNA-mediated crystallization of nanoparticle arrays into three-dimensional ordered structures; the production of hollow protein nanotubes by self-assembly of surface-modified hexameric ring structures; the deposition of metallic nanoparticles on a preapplied film of carbon nanotubes on plastic to create flexible hydrogen sensors; potential on-off switch for nano-electronics using mechanically controlled conductance of a single-molecule junction; improved hybrid solar cells via *in situ* ultra-violet polymerization.

### **Mission Relevance**

A part of the mission of the Office of Science is to "deliver the premier tools of science to our Nation's research enterprise." The NSRCs join the suite of major DOE user facilities that fulfill this objective. A seminal DOE-BES workshop and subsequent report on *Basic Research Needs to Assure a Secure Energy Future* cited nanoscience as a critical cross-cutting theme, and this has been reiterated in numerous follow-up reports on Basic Research Needs for specific focused

aspects of energy research, such as the hydrogen economy, solar energy utilization, and solid-state lighting. In addition, BES and the NSTC co-sponsored a major workshop and report on *Nanoscience Research for Energy Needs* that identified key research targets and foundational themes for energy-related nanoscience. As stated in the Executive Summary of that report, “At the root of the opportunities provided by nanoscience to enhance our energy security is the fact that all of the elementary steps of energy conversion (e.g., charge transfer, molecular rearrangement, chemical reactions, etc.) take place on the nanoscale.”

### **Scientific Challenges**

Strategic investments in scientific areas of opportunity are necessary to help our nation develop a balanced research and development infrastructure, advance critical research areas, and nurture the scientific and technical workforce of the 21<sup>st</sup> century. Nanotechnology R&D is a top federal priority with broad potential implications for the nation's competitiveness. DOE's participation in this effort includes the development and operation of the NSRCs, whose goals include: (1) to attain a fundamental scientific understanding of nanoscale phenomena, particularly collective phenomena; (2) to achieve the ability to design and synthesize materials at the atomic level to produce materials with desired properties and functions; (3) to take full advantage of other existing major user facilities, and (4) to develop experimental characterization techniques and theory/modeling/simulation tools necessary to drive the nanoscale revolution.

There are a large number of specific scientific challenges, many of which benefit from the collocation of disparate disciplines in order to fabricate, assemble, and otherwise manipulate nanosized components. One of the most challenging scientific problems is interfacing hard and soft matter, i.e., the world of electronic and structural materials with the world of biomaterials. These centers employ advanced experimental and theoretical tools to tailor and control the functionality (e.g., detection ability and sensitivity), compatibility, performance, and integration of materials at such interfaces.

### **Projected Program Evolution**

The NSRCs have completed the transition to standard user operations within the new facilities and with their initial suite of specialized technical equipment. This process brought major new resources on-line for users, including nanoprobe beamlines at synchrotron radiation sources, extensive cleanroom facilities, nanoscale electron beam writers, and extensive nanomaterials synthesis and assembly capabilities. User programs are adapting to respond to the needs of the community, with targeted acquisitions of new capital equipment and allocation of staff and accompanying resources to those areas that are most in demand. While a substantial user base is established already, the NSRCs are still being assimilated into the national scientific infrastructure; there will continue to be an increase in submitted proposals with a corresponding increase in users and/or corresponding decrease in the proposal approval rate, until a steady state is reached. The NSRCs are expected to perform as world-leading institutions, excelling both in scientific impact and productivity and in working with users. These are the fundamental criteria for evaluation of the NSRC facilities; each has undergone an initial (baseline) operations review and subsequent reviews will follow triennially.